

# Energy systematics of heavy nuclei – mean field models in comparison

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## Abstract

We compare the systematics of binding energies computed within the standard and extended versions of the relativistic mean-field (RMF) model and the Skyrme Hartree-Fock (SHF) model. The general trends for the binding energies for super-heavy nuclei are significantly different for these models. The SHF models tend to underbind the superheavy nuclei, while, RMF models show just the opposite trend. The extended RMF model seems to provide remarkable improvements over the results obtained for the standard RMF model.

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## I. INTRODUCTION

Self-consistent mean field (SCMF) models are the most feasible means for the microscopic description of ground state properties and low-energy collective dynamics of nuclei. These models are also employed for the study of compact stars, since they can be easily extended to include the contributions from hyperons and exotic phenomena as, e.g., kaon condensation [1, 2]. The three most prominent SCMF models are the Skyrme Hartree-Fock approach (SHF) [3, 4], the Gogny force [5], and the relativistic mean field model (RMF) [6–8]. We shall focus on SHF and RMF in comparison. SHF, as the name suggest, is based on the Skyrme energy functional derived from a zero-range effective interaction. The RMF models are based on an effective Lagrangian density which describes the interactions of nucleons through the exchange of the scalar-isoscalar ( $\sigma$ ), vector-isoscalar ( $\omega$ ) and vector-isovector ( $\rho$ ) meson fields.

The form of the energy functional or Lagrangian density is given by invariance constraints and plausible physical arguments (as, e.g., low-momentum expansion [3, 4, 9]). However, the parameters of the models are free parameters. A strict derivation from a microscopic nucleon-nucleon interaction has not yet been too successful at a quantitative level because ab-initio models, in spite of the enormous success over the last years, have still a limited quality if one refrains from adding empirical corrections like a three-body force (see, e.g., [10–12]). One of the important tasks in the development of mean field models is thus to devise ways of constraining the free parameters of interaction used. This is done usually by an adjustment to empirical data. This is, however, rather involved as one does not have a one-to-one correspondence between individual parameters and a specific piece of experimental information. Some parameters are well fixed by known nuclear ground state properties. Others remain only loosely determined leaving leeway for additional data or bias. Therefore, many tens of different parameter sets for SHF and RMF have evolved in the course of the development. A key task is to figure out which features depend on a particular parameterization and which features are more related to the intrinsic structure of the model. Recent extensive explorations of the SHF functional have indicated a few of such intrinsic features [13, 14]. One key problem is that all SHF functionals show a systematic trend to underbinding for super-heavy elements while traditional RMF parameterizations show an opposite trend to overbinding. It is the aim of the present contribution to study this discrepancy in more detail, in particular with more data and for a broader selection at the side of the RMF. To this end, we shall compare the binding energy systematics for even-even nuclei computed using the

standard and extended versions of the RMF models and the SHF models.

The RMF can be grouped into three different classes: (1) models with non-linear meson self-coupling [6], (2) models with density-dependent nucleon-meson coupling [15, 16], (3) models which combine (1) and (2). We concentrate here on class (1). Within these non-linear RMF one can distinguish two sub-classes: (i) standard RMF which includes the contributions from the non-linear self-couplings for the  $\sigma$  meson field only, and (ii) extended RMF model which includes the contributions from the self and/or cross interaction terms for the  $\sigma$ ,  $\omega$  and  $\rho$  meson fields. We will discuss both versions of meson coupling.

## II. CHOICES FOR THE MODELS

We have considered four different forces for both the RMF and SHF models. The specific reasons for choosing these forces are as follows. In particular, we employ the RMF parameterizations: NL3 [17], TM1 [18], FSUGold [19], and BSR4 [20, 21]. The non-linear part of the Lagrangian density for these RMF models are not the same. These differences are summarized in Table I. The Lagrangian density associated with the parameter set NL3 which represents the standard RMF model contains non-linear term only for the  $\sigma$  meson self-interaction. The Lagrangian density corresponding to the parameter set TM1 is extended to include the self-interaction term also for the  $\omega$  mesons. The FSUGold parameter set further includes the  $\omega - \rho$  cross-interaction term. The Lagrangian density corresponding to the BSR4 parameter set includes all the cross-interaction terms for  $\sigma$ ,  $\omega$  and  $\rho$  mesons up to quartic order, but, the self-interaction of the  $\omega$ -meson is switched off. These parameter sets should enable us to delineate the effects of the meson self- and cross-interactions on the binding energy systematics. We neglect the contributions from the self interaction of  $\rho$  mesons as they can affect the properties of the finite nuclei and neutron stars only marginally [22].

At the side of SHF, we consider the following four parameterizations: SkI3 [23], SLy6 [24], BSk4 [25] and SV-min [13]. The form of the SHF functional is basically the same for all four cases with the tiny difference that SkI3 and SV-min include an isovector contribution to the spin-orbit term [23]. The parameterizations differ mainly in the bias and choice of data for the phenomenological adjustment. The two older parameterizations SkI3 and SLy6 used a rather small set of fit nuclei. SkI3 included the electro-magnetic form factor and isotope shifts as data while SLy6 put emphasis on the neutron rich side and included data from bulk matter. BSk4 puts emphasis

almost exclusively on binding energies, and includes all known even-even nuclei in the data base. SV-min takes a data set of good “mean-field nuclei” which were carefully selected to contain only negligible corrections from collective correlations [26]. This amounted to long chains of semi-magic nuclei. The fit set is much larger than the one for SkI3 and SLy6, but much smaller than for BSk4. On the other hand, SV-min takes care not only of binding energies but of a larger set of observables (radii, electro-magnetic form factor, spin-orbit splittings, ...). The four selected forces are thus sufficiently different with respect to these aspects of bias and choice.

We would like to briefly outline the manner in which the corrections to the binding energies arising from the centre of mass motion, pairing and quadrupole correlations are incorporated. All models include the correction for the spurious center-of-mass energy  $E_{\text{cm}}$ . The SHF sets compute it from,

$$E_{\text{cm}} = \langle \hat{P}_{\text{cm}}^2 \rangle / (2mA), \quad (1)$$

while the RMF sets use the estimate

$$E_{\text{cm}} = 31 A^{-1/3} \text{ MeV}. \quad (2)$$

The values of  $E_{\text{cm}}$  computed using Eqs. (1 and 2) for the cases with mass number  $A \geq 200$ , which is of present interest, may differ at most by  $\sim 0.5$  MeV [27]. The pairing is treated within the SHF models using a (density dependent) zero-range force and smooth cutoff in pairing space [28–30]. For the RMF models, the contributions from the pairing correlations to the binding energy are evaluated in the constant gap approximation with the gap [31],

$$\Delta = \frac{11.2}{\sqrt{A}} \text{ MeV}. \quad (3)$$

Soft nuclei and deformed nuclei can develop substantial contributions from quadrupole correlations [26]. As an efficient and simple estimate we include a large part of these correlations in terms of approximate rotational projection expressed through variance of total angular momentum  $\langle \hat{J}^2 \rangle$  and moment of inertia  $\Theta$  [26, 32]. This is done so far for the SHF models. In case of RMF, we use a simple estimate for the quadrupole correlation energy or rotational correction as,

$$E_{\text{rot}} = 2.2 \sqrt{\beta_2 - 0.05} m/m^* \text{ MeV} \quad (4)$$

where  $m^*$  is the nucleon effective mass in bulk equilibrium matter. This estimate has been extracted by studying the microscopically computed trends of  $E_{\text{rot}}$  for a wide variety of SHF parameterizations. Thus, the manner in which the contributions from the c.m. correction  $E_{\text{cm}}$ , from the pairing

correlations and from the rotational correction  $E_{\text{rot}}$  to the binding energy evaluated for the SHF and the RMF models are not exactly the same. We have checked these variants extensively and found that they do not affect the general trends which we aim to discuss. To this end, we may point out that the contributions from the Fock and the Coulomb exchange terms are ignored in the RMF models, but, included in the SHF models.

### III. BINDING ENERGY SYSTEMATICS

We first present some numerical details before embarking on our main results. The RMF equations for nucleons are solved by expanding the Dirac spinors in terms of the wave functions for the axially deformed harmonic oscillator potential [33, 34]. Similar strategy is employed for solving the field equations for the mesons. The basis space for the nucleons and the mesons are truncated at the major oscillator shells  $N_F$  and  $N_B$ , respectively. The reliable solutions for the field equations can be obtained with  $N_B = 10$  [33]. However, the appropriate choice of  $N_F$  depends on the mass number of the nucleus. For instance, reliable binding energy for  $^{208}\text{Pb}$  requires number of oscillator shells  $N_F \geq 12$ . It is quite natural to expect the need for larger basis space for the case of superheavy nuclei which are also well deformed in general. Our prime interest is to look into the binding energy systematics of the superheavy nuclei, it is therefore necessary to ensure that the basis space used is sufficiently large enough to yield meaningful values for the binding energies for these nuclei. In Figs. 1 and 2 we display the results for the binding energy error or equivalently the mass difference between the measured and the calculated ones,

$$\delta M = M_{\text{exp}} - M_{\text{th}} \quad (5)$$

as a function of  $N_F$  for some heavy nuclei. The values of  $E_{\text{rot}}$  as used for the results plotted in Fig. 2 are obtained from Eq. (4). It can be seen from these figures that we need at least  $N_F = 18$  to generate reliable binding energy systematics over wide range of mass number. In Table II we compare our results for the binding energies for a few selected nuclei with those of Ref. [35] obtained for  $N_F = 12$ . We see that our results obtained with the  $N_F = 12$  agree reasonably well with those of Ref. [35]. Though, the pairing gaps used in our paper may be somewhat different. Large differences in the binding energy for the super-heavy nuclei in our work as compared to that of Ref. [35] are mainly due to the fact that we have used sufficiently large basis space (see also Figs. 1 and 2). All the results obtained within the RMF models as presented below correspond to

$N_F = 18$  with  $N_B = 20$ .

In Fig. 3 we summarize the errors in binding energies (Eq. 5) for all experimentally known even-even nuclei. The upper block collects the results from RMF and the lower block those from SHF. As a first impression we note the rather small energy scale of a few MeV for the error plots. All parameterizations shown here provide a good description of known nuclei in the mass range  $A = 16 - 220$ . There are, of course, differences in detail to the extent that in each block the most recent parameterizations perform visibly best. This concerns BSR4 in the RMF block and BSk4 as well as SV-min in the SHF block. We have indicated the present “state of the art” by  $\pm 1$  MeV error bars and these three most recent parameterizations stay close to this goal. It is also found as a general rule that robust spherical nuclei, denoted as “fit nuclei” in most parameterizations, are usually somewhat better described than soft or deformed nuclei. At this point it is important to emphasize that the still good description of soft and deformed nuclei is achieved only with the rotational correction and one may reduce the error even more by performing the full collective correlations [26]. We also calculate the rms error for the binding energies using the results for all the 513 even-even nuclei as considered in the present work. These rms errors as given in the parenthesis in the units of MeV are: BSR4(2.6),FSUGold(6.5),NL3(3.8),TM1(5.9),SV-min(1.6),BSk4(1.1),SkI3(2.6),SLy6(2.3). Our rms error for the case of BSk4 is higher than  $\sim 0.6$  MeV [25]. Because we use different rotational correction, which probably has some effect for deformed nuclei. Moreover, the basic paper for the BSk4 force uses a different recipe for the cutoff of the pairing space. Their pairing band amounts to 15 MeV while we stay typically in the range of 5 MeV. That could have a some effect on heavy nuclei. Nevertheless, it may be emphasized that these differences in detail do not change the gross trends for the binding energy errors. In particular trends for the binding energy errors for the super-heavy nuclei presented in Fig. 3 are very much similar to those of Ref. [25].

Having a closer look at the trends with mass number we see in all cases a growing deviation from the zero line with increasing mass number. This trend shown here on a much larger data basis confirms what had been observed in [13], namely that SHF drives to underbinding of super-heavy nuclei while RMF shows just the opposite trend. This trends become manifest in the region  $A > 220$ , but develop already for deformed nuclei in the region  $150 < A < 220$ . Within the SHF parameterizations there are significant differences in the quantitative level of the deviation. BSk4 manages best to minimize the unwanted trend, achieved through the strong bias on binding energies, however, other observables are compromised. In the realm of the RMF the trend to

overbinding is even more dramatic. This is obvious in the traditional RMF, parameterization NL3 in figure 3. Somewhat surprisingly, the situation does not improve with  $\omega$  self-couplings in TM1 and the one more cross coupling in FSUGold. It is only BSR4 having the isoscalar and isovector cross-couplings with the  $\sigma$  fields which allows to produce a much better overall trend in binding energies. These couplings seem to be a crucial ingredient for success and it is to be noted that SHF contains them in the isoscalar and isovector density-dependent terms.

We have looked into the possible consequences of the approximations used in the present work to evaluate the pairing and quadrupole correlation energies for the RMF cases. In Fig. 4, we plot the SHF results for the errors in the binding energies obtained for the SV-min and SkI3 forces. For both the cases, the pairing and quadrupole correlation energies are calculated approximately using Eqs. (3) and (4), respectively. Comparing these results with the corresponding ones as shown in lower block of Fig. 3, which are obtained by treating the pairing and quadrupole correlations microscopically, we find that the approximations used to evaluate the pairing and quadrupole correlation energies do not affect the global trends. Finally, we compare our results for the BSR4 force for a few heavy nuclei with those obtained using the density dependent meson exchange, DDME2, force [36]. It appears that the BSR4 and DDME2 forces yield similar trends for the binding energy errors for the heavy nuclei.

Comparing the three best performers, BSR4, BSk4 and SV-min, we see that both models are approaching good control over the energies for super-heavy elements. And yet, there remains an unresolved trend which still is distinctively different between SHF and RMF. The reasons for that are not yet clear. We try briefly to sort out possible mechanisms. The defect seems to come from the deformation energy because the large deviation develops with deformation. This, in turn, localizes the differences in the modeling of the surface energy, and most probably isovector surface energy (also called surface symmetry energy) because heavier nuclei have naturally a larger asymmetry. A direct relation between surface energies and model parameters has not yet been established [37]. At present we can only speculate and try to figure out the terms which could have an influence. Although one can map at lowest order  $v/c$  the RMF into a Skyrme-like functional including proper kinetic and spin-orbit terms [38], there remain basic differences between the two classes of models. The spin-orbit and kinetic terms in the RMF carry effectively a strong density dependence while the corresponding SHF terms stay simply linear in  $\rho$ . This yields a different performance with respect to spin orbit splitting and a different density profile in super-heavy elements [39], which both are possible sources for different deformation energies.

Moreover, the RMF produces a strong link between effective mass and spin-orbit force where one of the consequences is that RMF models produce typically very low effective masses in the range  $m^*/m \approx 0.6$  while SHF has much more freedom in the effective mass and in adjusting the spin-orbit term independently. It is certainly a worthwhile task for future work to find out the mechanisms determining the trends as it will shed light on the structure of both approaches, SHF and RMF, and indicate missing pieces in the functionals.

#### IV. SUMMARY

In summary, we have calculated the binding energies, for all experimentally known even-even nuclei, within the RMF and the SHF models. For the RMF models, we have used four different parameter sets corresponding to different functional forms for the non-linear part of the Lagrangian density. The NL3 parameterization corresponds to the Lagrangian density associated with the standard RMF model. While the Lagrangian density for the TM1, FSUGold and BSR4 parameterizations correspond to the extended RMF model which include contributions from the self-interaction of the  $\omega$  meson and/or the cross-interaction between  $\sigma$ ,  $\omega$  and  $\rho$  mesons (see Table I). For the SHF model we have used four parameter sets, namely, SkI3, SLy6, BSk4 and SV-min. The form of the SHF functional is basically the same for all four cases with the tiny difference that SkI3 and SV-min include an isovector contribution to the spin-orbit term [23]. We find that all parameterizations of the RMF and SHF model considered provide a good description of known nuclei in the mass range  $A = 16 - 220$ . There are, of course, differences in detail to the extent that the most recent parameterizations perform the best. These parameterizations are BSR4 in the RMF model and BSk4 as well as SV-min in the SHF model.

The binding energies for the super-heavy nuclei ( $A > 220$ ) for the RMF and SHF models are significantly different from the experimental data. The SHF drives to underbinding of super-heavy nuclei while RMF shows just the opposite trend. This trend on a much larger data basis confirms what had been observed in [13]. The absolute errors in the binding energies for the extended RMF model (BSR4) which includes contributions from all the cross-interaction terms are comparable to that for the SHF models. Other RMF models considered yield much larger values for the absolute errors in the binding energies for the super-heavy nuclei.

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TABLE I: Various self-interaction and cross-interaction terms present in the Lagrangian density associated with different parameterizations of the RMF models. The index '1' and '0' is used to indicate whether or not the corresponding term is included.

	Self-interaction			Cross-interaction		
	$\sigma$	$\omega$	$\rho$	$\sigma-\omega$	$\sigma-\rho$	$\omega-\rho$
NL3	1	0	0	0	0	0
TM1	1	1	0	0	0	0
FSUGold	1	1	0	0	0	1
BSR4	1	0	0	1	1	1

TABLE II: Comparison of our results for the binding energies (in MeV) for the NL3 force with the corresponding ones given in Ref. [35].

Nucleus	Ref. [35]	This work	
	$N_F = 12$	$N_F = 12$	$N_F = 18$
O16		128.82	128.84
Ca40	341.91	341.96	341.99
Ca48	415.07	415.11	415.06
Ni58	503.54	503.39	503.08
Zr90	783.41	783.08	783.06
Sn116	986.44	986.15	986.79
Sn124	1048.58	1048.15	1048.49
Sn132	1104.72	1104.81	1104.77
Pb208	1640.16	1640.30	1640.50
Pb214	1662.70	1662.02	1662.52
Th232	1764.99	1764.12	1767.33
Cf248	1857.17	1856.48	1861.51
Hs264		1927.95	1934.68

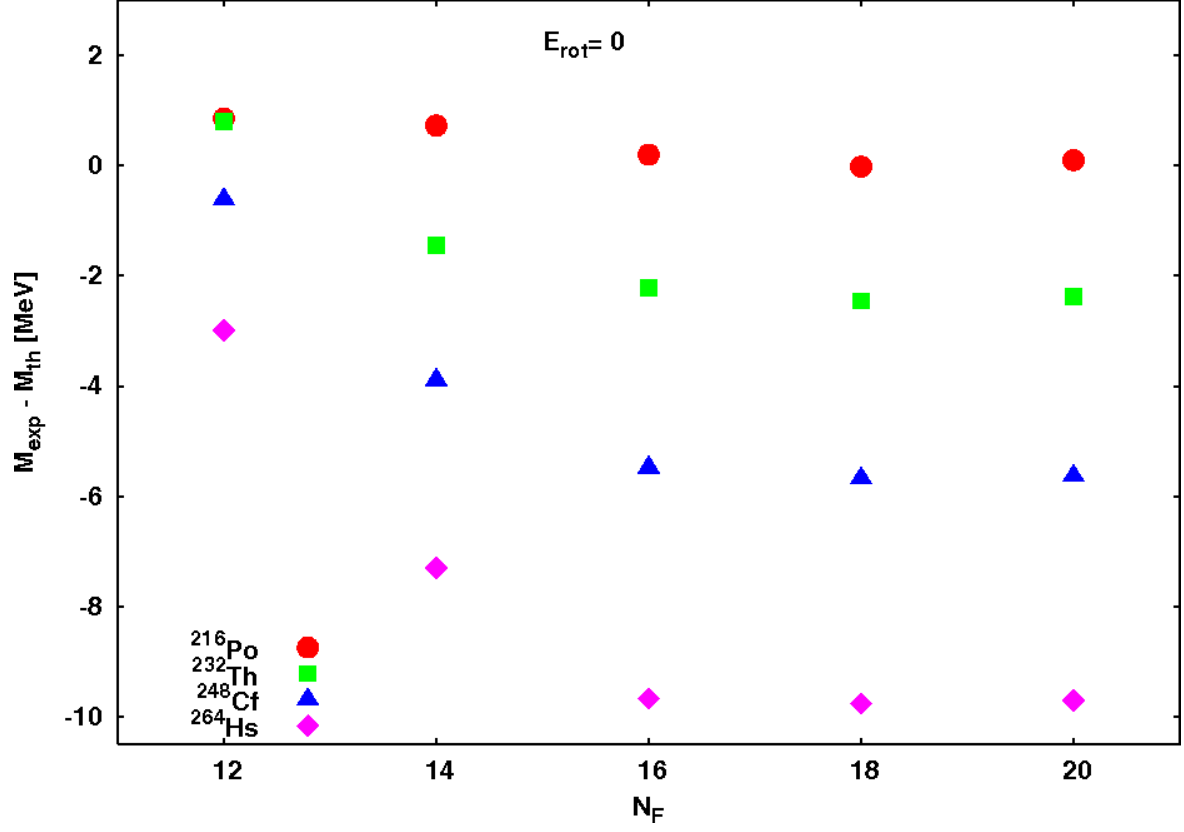


FIG. 1: (color online) Errors in the binding energy (Eq. 5) plotted as a function of the number of oscillator shells  $N_F$  employed to expand the Dirac spinors for nucleons.

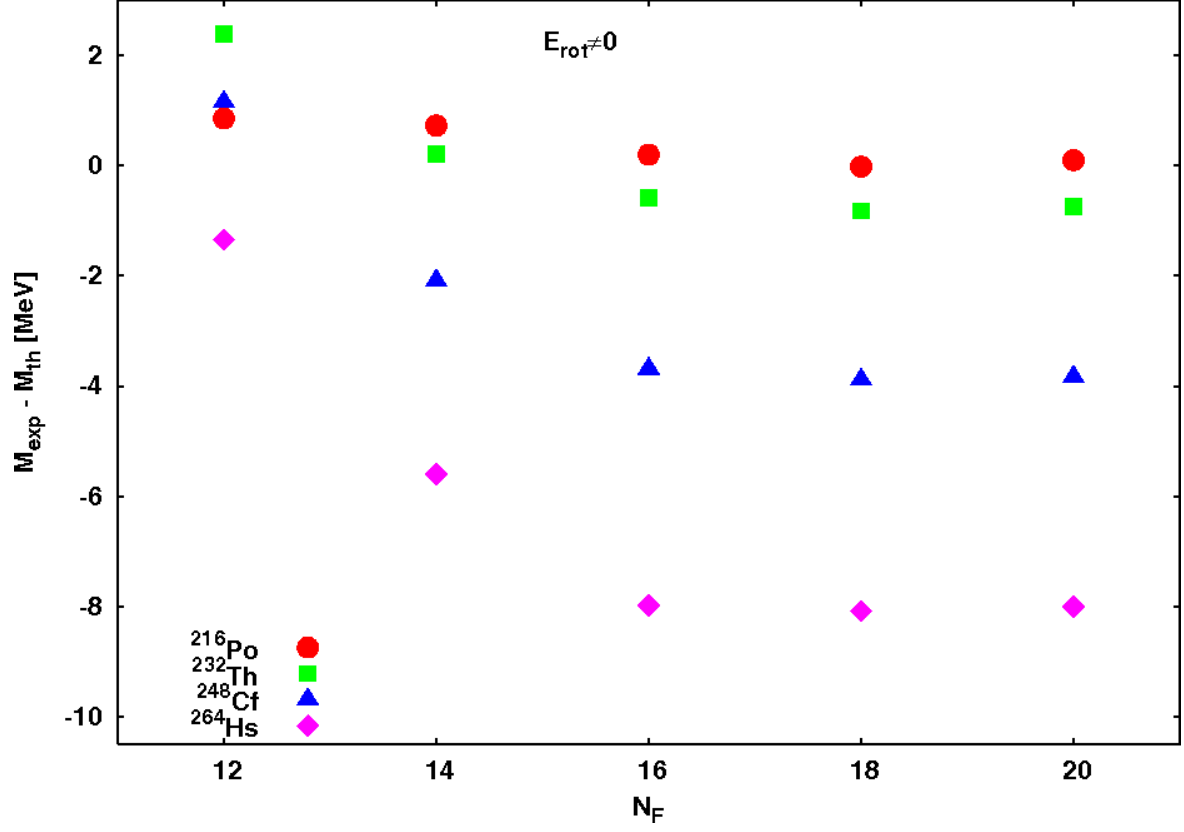


FIG. 2: (color online) Same as Fig. 1, but, the quadrupole correlation corrections also included (Eq. 4).

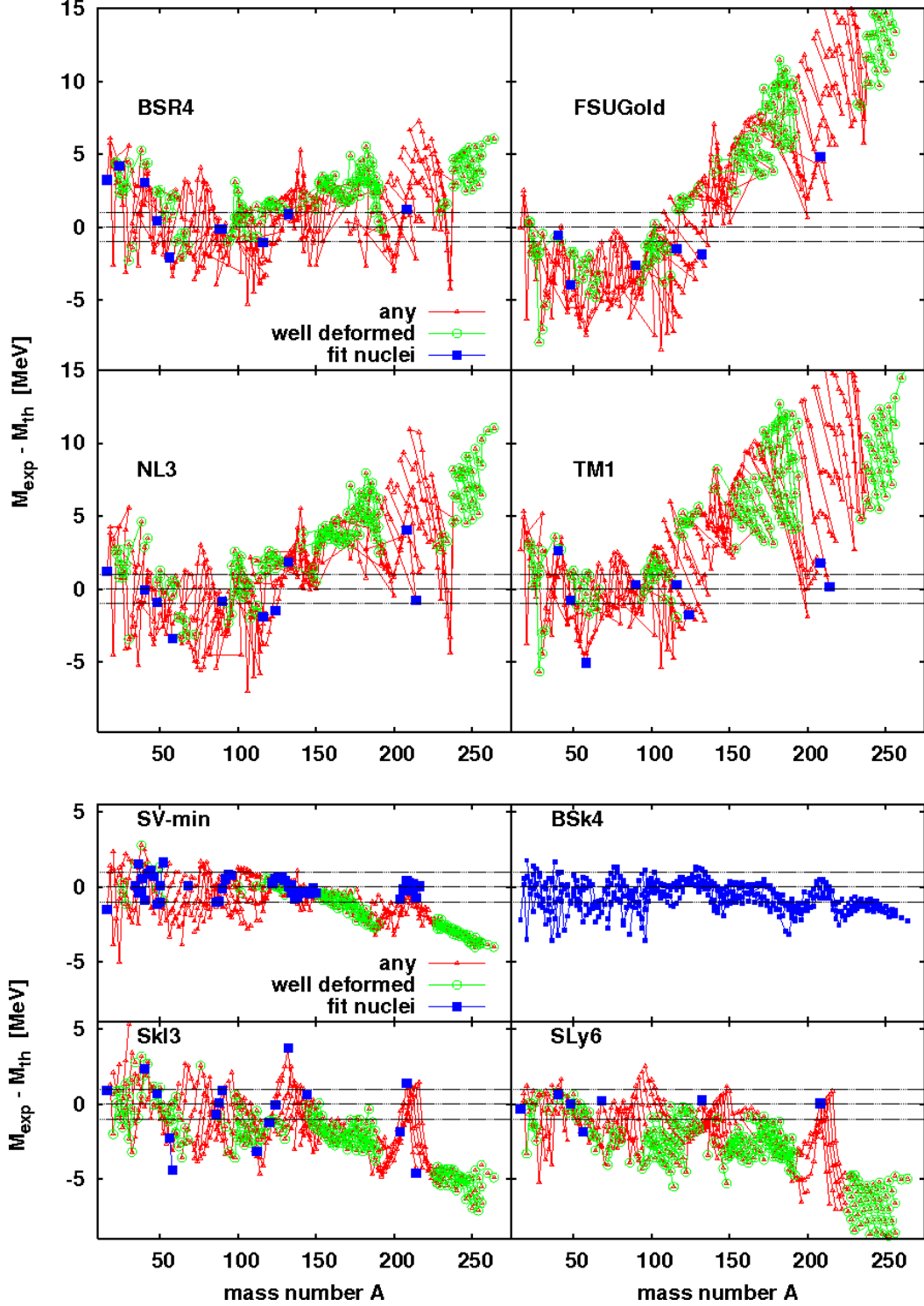


FIG. 3: (color online) Errors in the binding energy versus the mass number obtained for different parameterizations of the RMF (upper block) and SHF (lower block). The nuclei that were included in the fit are marked by filled squares, well-deformed nuclei by open circles, and all others by triangles. Binding energy error equal to zero and  $\pm 1$  MeV are indicated by faint horizontal lines. The corrections to the binding energies due to the pairing and quadrupole correlations are included for all the cases (see text for detail).

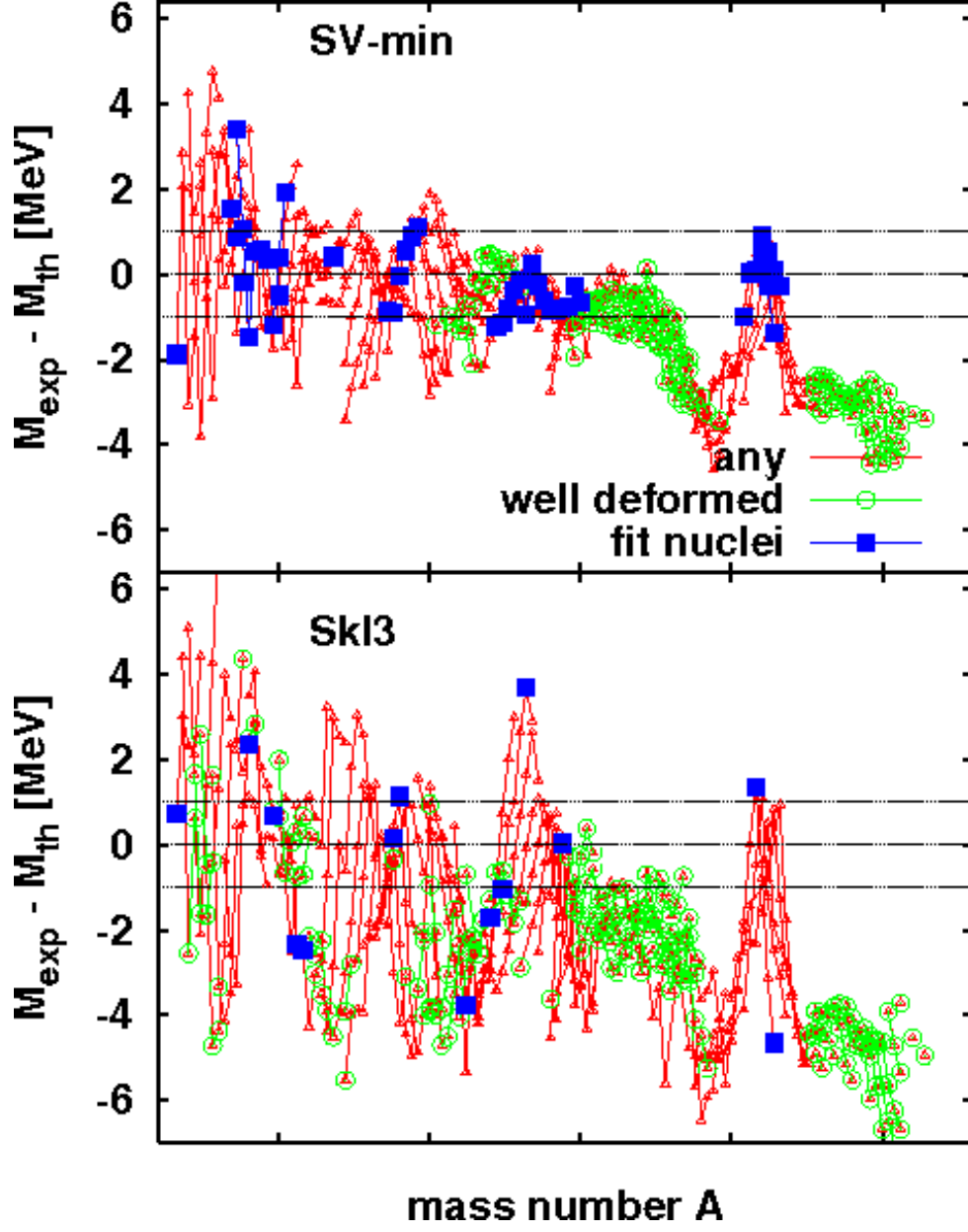


FIG. 4: (color online) Errors in the binding energies verses the mass number  $A$ . The corrections to the binding energies due to the pairing and quadrupole correlations are evaluated approximately using Eqs. (3) and (4).



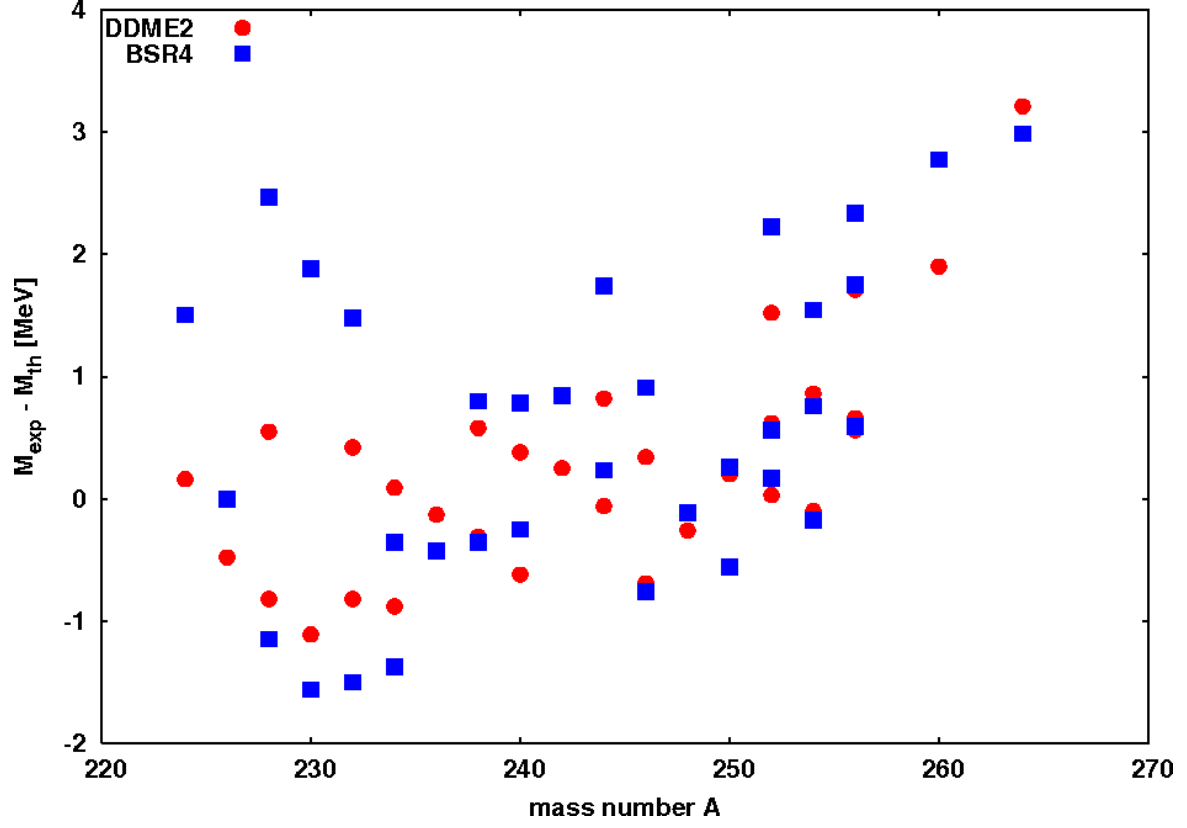


FIG. 5: (color online) Comparison of the binding energy errors for the BSR4 force with those for the DDME2 force for a few superheavy nuclei.